

Supporting Information

Mechanisms for the Insertion of Toxic, Fibril-like β -Amyloid Oligomers into the Membrane

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Title Running Head: Membrane insertion of Alzheimer's toxic A β oligomer

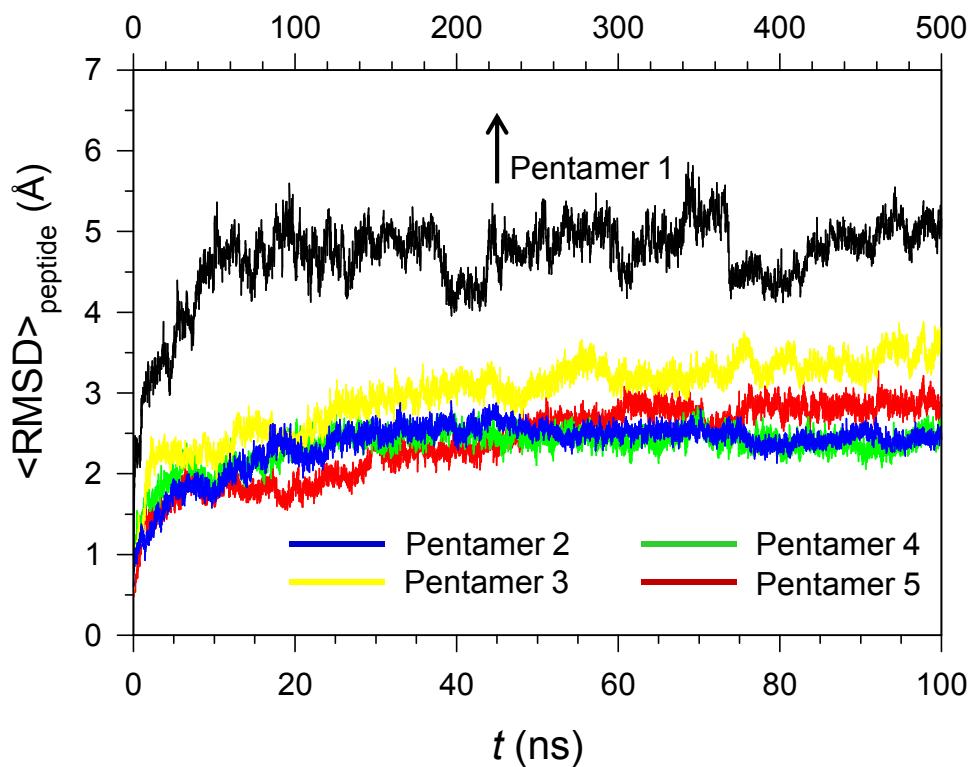


FIGURE S1. The root-mean-squared deviation (RMSD) from the starting point for backbone heavy atoms averaged over the peptides in the p3 ($\text{A}\beta_{17-42}$) pentamers.

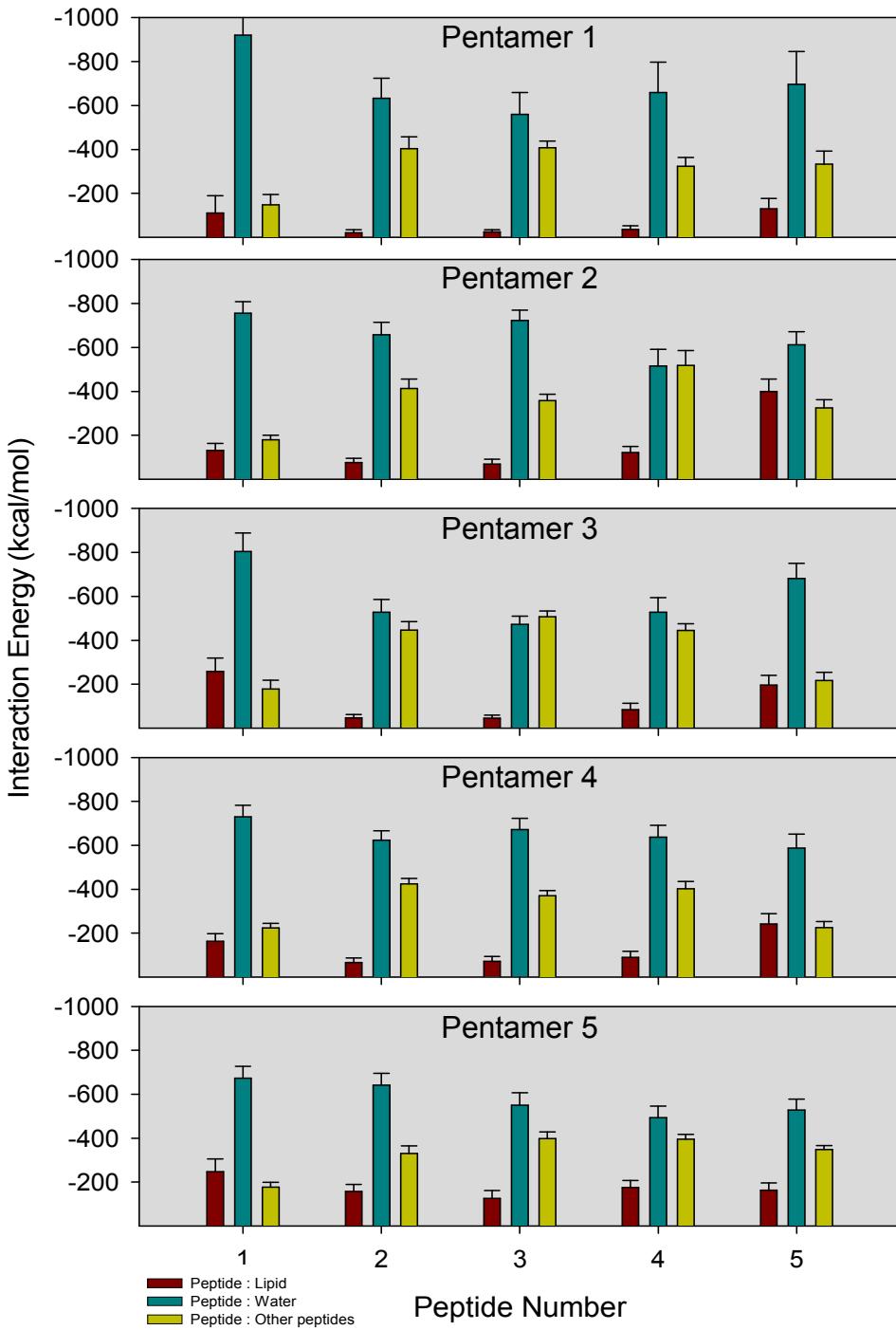


FIGURE S2. Interaction energies of each monomer in the p3 ($\text{A}\beta_{17-42}$) pentamers. All peptide-lipid interactions were calculated separately for the peptides interacting with DOPC lipids, waters, and other peptides.

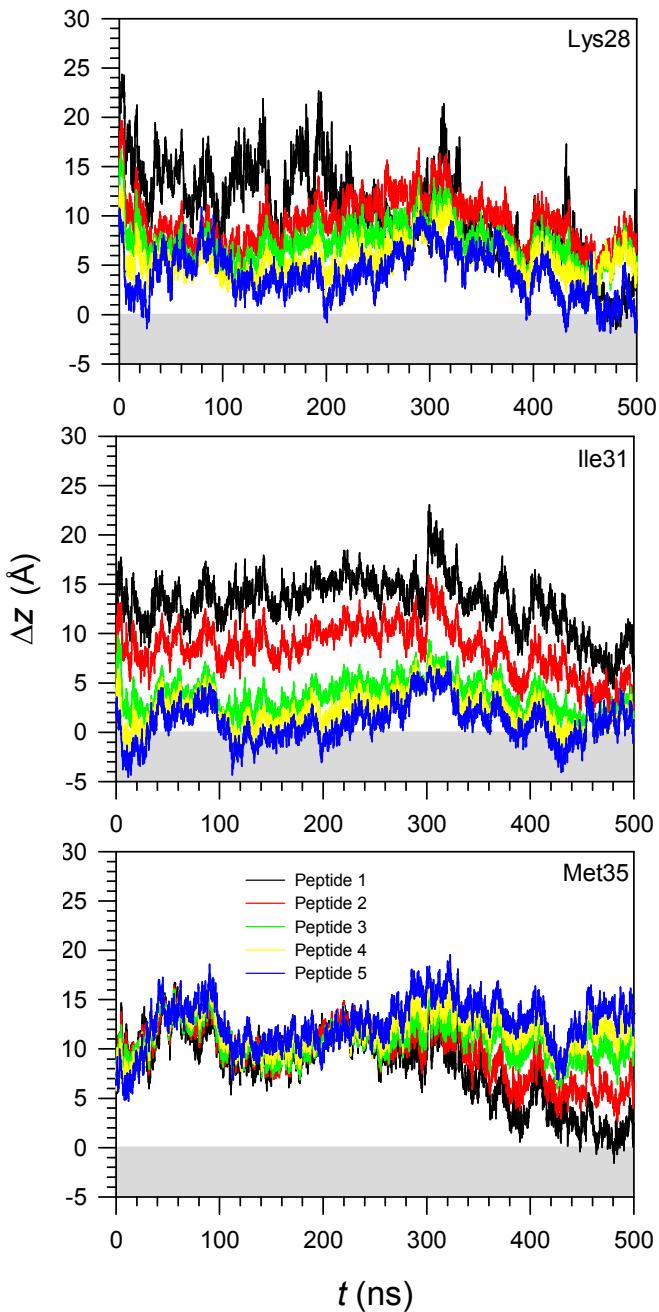


FIGURE S3. Time series of the center of mass deviation, Δz , from the upper bilayer leaflet for the Lys28 (top panel), Ile31 (middle panel), and Met35 (bottom panel) residues of each monomer in the p3 ($A\beta_{17-42}$) pentamer in configuration 1. Light gray area denotes the amphipathic interface of the lipid bilayer.

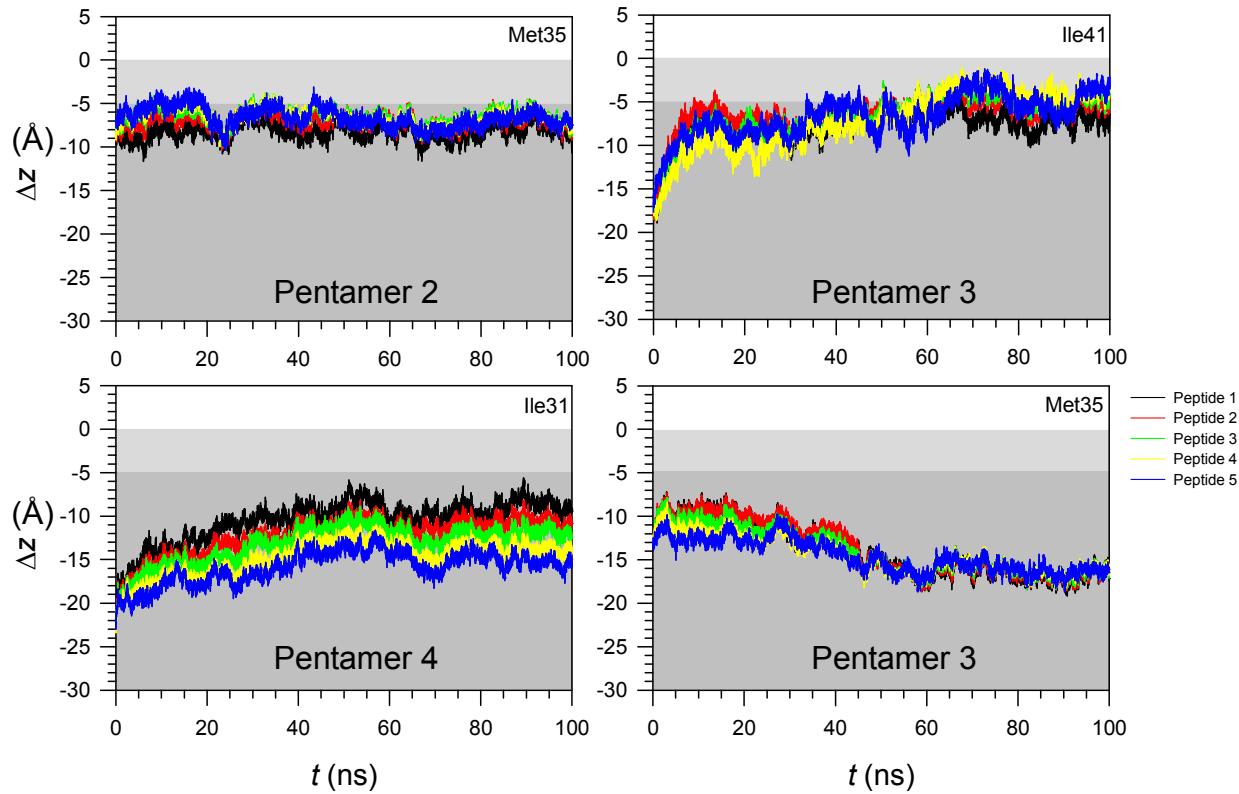


FIGURE S4. Time series of the center of mass deviation, Δz , from the upper bilayer leaflet for the Met35 (top left panel), Ile41 (top right panel), Ile31 (bottom left panel), and Met35 (bottom right panel) residues of each monomer in the p3 ($\text{A}\beta_{17-42}$) pentamers in configuration 2, 3, 4, and 5, respectively. Light and dark gray areas denote the amphipathic interface and the hydrophobic core of the lipid bilayer, respectively.

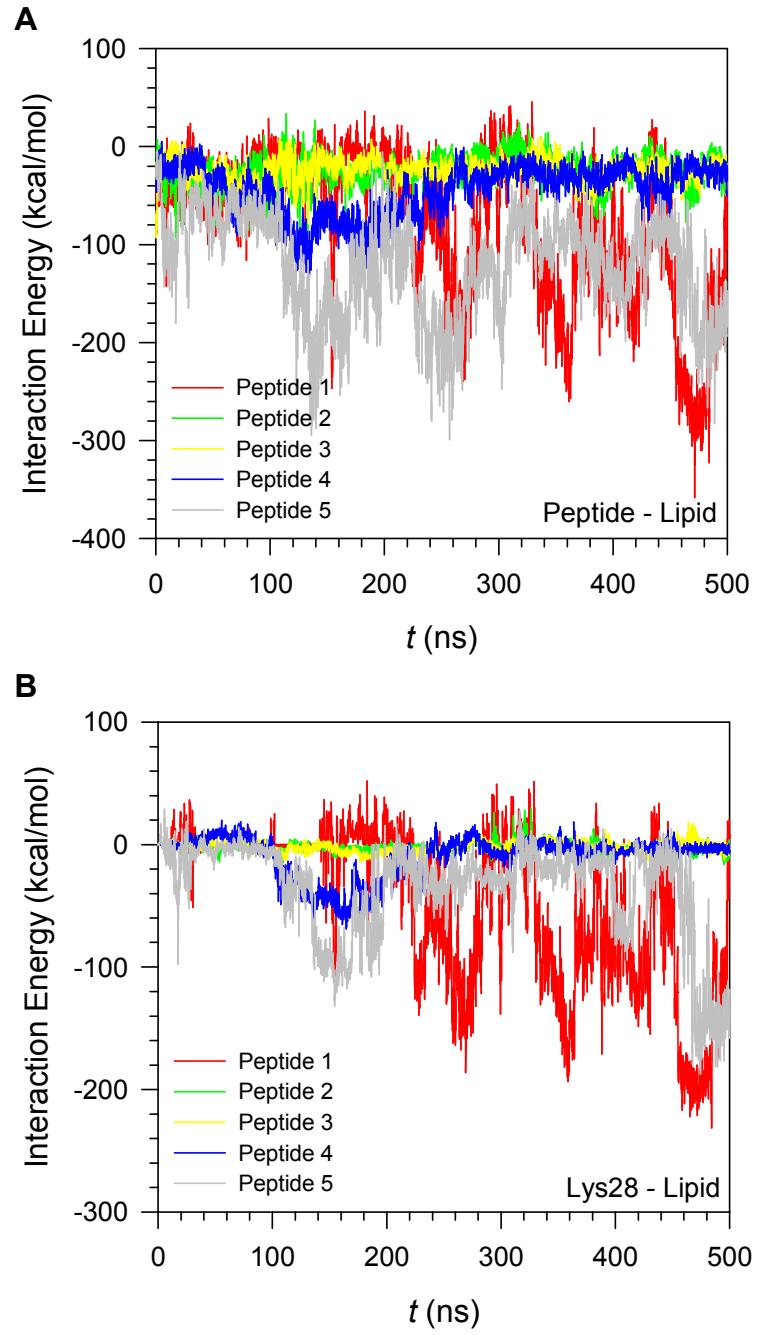


FIGURE S5. Time series of interaction energies of (A) each monomer and (B) the Lys28 residue in each monomer with DOPC lipids for the p3 ($\text{A}\beta_{17-42}$) pentamer in configuration 1.

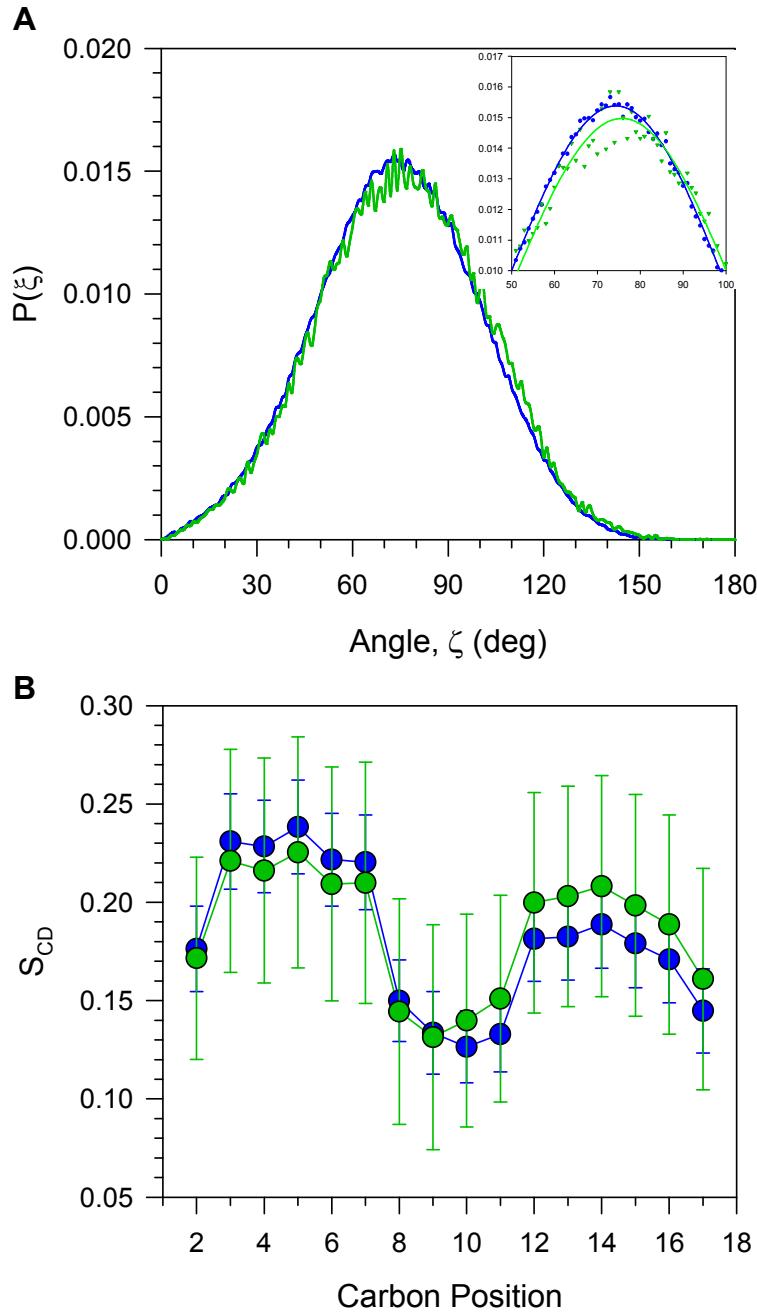


FIGURE S6. (A) Probability distribution, $P(\xi)$, of the angle between the P-N vector, where P and N denote the phosphate and nitrogen atoms in lipid headgroup respectively, and the bilayer normal for the p3 ($\text{A}\beta_{17-42}$) pentamer in configuration 1. Blue curve representing the distribution for the lipids located far from the pentamer shows a peak at the typical ξ value for the PC lipid head, while green curve for the lipids nearby the pentamer within 10 Å cutoff show a peak at slightly higher ξ value indicating disordered lipid heads. Inset highlights the peaks with smooth lines representing data regression. (B) Deuterium order parameters, S_{CD} , for the tails of DOPC lipids located far from (blue symbols) and nearby (green symbols) the p3 ($\text{A}\beta_{17-42}$) pentamer in configuration 1.